



**UNIVERSITY OF LEEDS**

## **CANDIDATE BRIEF**

**KTP Associate – Scientific Software Developer for Digital Design of Pharmaceutical Products, Faculty of Engineering and Physical Sciences, and The Cambridge Crystallographic Data Centre**



**Salary: £30,000 – £33,000 plus training allowance of £5,600. This position is not on the University of Leeds salary scale.**

**Reference: CSRIS1140**

**Based at the company premises in Cambridge**

**Fixed term for 34 months due to external funding for a fixed period.**

**This post is advertised subject to funding.**

# KTP Associate – Scientific Software Developer for Digital Design of Pharmaceutical Products

## School of Chemical and Process Engineering and The Cambridge Crystallographic Data Centre (CCDC)

**Do you have a PhD in science, mathematics or computer software development (or equivalent experience)? Do you have experience of writing scientific code in C++ or a similar language? Are you keen to apply your academic achievements to industry-ready products?**

We have an opportunity for you to ‘fast track’ your career in industry by leading a strategically important project to a successful conclusion. Through a [Knowledge Transfer Partnership](#) (KTP), you will be working in partnership with [The Cambridge Crystallographic Data Centre \(CCDC\)](#) and the [School of Chemical and Process Engineering](#) at one of the UK’s leading research intensive universities. You will have an excellent opportunity to utilise your academic achievements in an industry setting. The CCDC is an independent not-for-profit organisation with world-leading expertise in chemical and crystal structure data. They are leaders in the development of software for solid state chemistry, working closely with many of the world’s top pharmaceutical companies.

This project aims to develop and bring to market a state-of-the-art digital design platform to automate, streamline and accelerate the design, development and manufacturing of pharmaceutical products.

A major challenge in the pharmaceutical sector currently is the lack of suitable digital platforms for drug development and manufacturing, as well as the adoption of these methods. CCDC’s long term strategic objectives are to address this through embedding use of their tools and expertise across the pharmaceutical industry, from discovery through development to delivery. A particular goal is to reduce pharmaceutical development times to enable access to and reduce costs for new drugs.

This project presents an opportunity to excel in an interdisciplinary project that combines chemical & process engineering, software development and business development including real-life application of expert knowledge to industry-ready products.





You will be based at the company premises in Cambridge, but will be employed by the University of Leeds for the duration of the project, a fixed period of 34 months, spending some of your time at the University of Leeds. The School of Chemical and Process Engineering will provide academic and technical support to you throughout the project, with business guidance and mentoring from the [Management Division of Leeds University Business School](#).

You will have access to a training and development package worth £5,600 to be spent according to your needs and the project's requirements, enabling you to work effectively on the KTP and to plan for your future career. Additionally, you will attend two weeks of residential KTP training to equip you with the skills and knowledge required to complete the project successfully, for which time is allocated and funding provided.

In addition to the challenges of the post, you will be expected to work towards a chartered membership of an appropriate professional body.

## What does the role entail?

The project comprises of two strands: software development and innovation management. Engagement with industry will enable product development informed by user needs and subsequent adoption through training and outreach.

As a KTP Associate, Your main duties will include:

- Establishing customer requirements and market analysis within the pharmaceutical industry;
- Establishing a steering committee comprising key pharmaceutical companies using CCDC's existing platform, the academic and company supervision teams and other key stakeholders, to aid adoption of the new Particle suite - a set of tools to provide insights into pharmaceutical formulation and manufacturing challenges;
- Engaging with key industrial users, tailoring outputs to the practical needs of industry – e.g. user experience, report generation, impactful visualisation;
- Developing existing algorithms for computing intermolecular interaction energies to process complex multi-component systems;
- Reimplementing and integrating legacy code developed over the past 30 years from FORTRAN77 to C++;



- Extending existing code to cope with a wider range of systems used in the real world;
- Using automated test frameworks to ensure the stability of the software along with validity and reproducibility of outputs;
- Writing technical documentation for future maintenance and support of the code;
- Delivering the new software suite, comprising a marketing strategy and embedding the knowledge within the business;
- Ensuring successful commercial exploitation and wider adoption of the new software suite by engaging with existing and potential user communities to establish industry use cases and provide feedback on R&D priorities;
- Developing user documentation, workshop/training material, case studies and white papers that highlight the capabilities of the new software suite;
- Identifying areas of applicability for software tools beyond the pharmaceutical sector;
- Presenting at conferences and submitting papers to quality publications;
- Team working and communication to identify opportunities and resolve issues;
- Disseminating and embedding knowledge and expertise with the CCDC Materials Science team and wider organisation, including through training and documentation.

These duties provide a framework for the role and should not be regarded as a definitive list. Other reasonable duties may be required consistent with the grade of the post.

## What will you bring to the role?

As a KTP Associate you will have:

- A PhD in Chemistry, Physics, or Chemical/Process Engineering, Mathematics or Computer Software Development, or equivalent experience;
- Experience of writing scientific code in C++ or another object-oriented language;
- Good code design skills such as object-oriented design;
- Appreciation of professional programming practices (source control, documentation, unit testing etc.);
- Excellent written and oral communication skills enabling communication within academia and industry, including with non-specialist scientists;



- Strong presentation skills;
- Desire and aptitude to learn additional concepts and technologies;
- Desire to develop business development skills in a commercial software development environment;
- Pro-active, self-motivated approach comfortable taking responsibility;
- A practical, pragmatic approach to work, with expert problem solving skills and good attention to detail;
- Strong initiative and a proactive approach, with excellent organisational, planning and self-management skills, including the ability to prioritise a complex workload to meet deadlines/demand and deliver high quality work under pressure;
- A desire to develop your career in a progressive company;
- Flexibility and a willingness to travel.

You may also have:

- Experience with Python;
- Appreciation of Agile development methodologies;
- Experience in structural chemistry or a related field.

## How to apply

You can apply for this role online; more guidance can be found on our [How to Apply](#) information. Applications should be submitted by the advertised closing date.

## Contact information

To explore the post further or for any queries you may have, please contact:

### **Dr Robert Hammond**

Tel: +44 (0)113 343 2428

Email: [R.B.Hammond@leeds.ac.uk](mailto:R.B.Hammond@leeds.ac.uk)

### **Professor Kevin Roberts**

Tel: +44 (0)113 343 2408

Email: [K.J.Roberts@leeds.ac.uk](mailto:K.J.Roberts@leeds.ac.uk)

### **Dr Andrew Maloney (CCDC)**

Tel: +44 (0)1223 336408





Email: [maloney@ccdc.cam.ac.uk](mailto:maloney@ccdc.cam.ac.uk)

## Additional information



Candidates must be available for an onsite interview at the company premises.

### Working as a KTP Associate

You will be employed by the University of Leeds and will have access to University facilities. However, you will be based for the majority of your time at the company premises, working to their terms.

You will have access to the University's USS pension scheme, with generous employer contributions.

### Faculty and School Information

Further information is available on the research and teaching activities of the [Faculty of Engineering and Physical Sciences](#) and the [School of Chemical and Process Engineering](#).

### A diverse workforce

The Faculty of Engineering is proud to have been awarded the [Athena Swan Silver Award](#) from the Equality Challenge Unit, the national body that promotes equality in the higher education sector. Our [equality and inclusion webpage](#) provides more information.

### Candidates with disabilities

Information for candidates with disabilities, impairments or health conditions, including requesting alternative formats, can be found in our [Accessibility](#) information or by getting in touch with us at [disclosure@leeds.ac.uk](mailto:disclosure@leeds.ac.uk).

The post is located at the company premises. Candidates with disabilities wishing to review access to the building are invited to contact Laura Dugdale (Research and Innovation Service), [L.Dugdale@Leeds.ac.uk](mailto:L.Dugdale@Leeds.ac.uk) or Tel: 0113 343 0928.



## Criminal record information

### Rehabilitation of Offenders Act 1974

A criminal record check is not required for this position, however, all applicants will be required to declare if they have any 'unspent' criminal offences, including those pending.

Any offer of appointment will be in accordance with our Criminal Records policy. You can find out more about required checks and declarations in our [Criminal Records information](#).

